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Key Issues in Modeling Indoor Air Quality for Building Design

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Because of its impact on the health and productivity of building occupants, indoor air quality (IAQ) should be an important consideration in the design of any building to be used by U.S. Army military personnel or civilian employees. Frequently, however, IAQ does not receive adequate attention during design because the interrelationships between IAQ and design are often too complex or subtle to be fully understood by the architect or engineer. An effective IAQ model could help the designer take into account the major elements that contribute to poor IAQ and understand the implications his or her design decisions may have on IAQ.

This report discusses key issues to be addressed in the development of an effective computer-based IAQ modeling system. The major indicators of an IAQ problem are outlined, and the contaminants that most commonly create such problems are identified. The state of modeling technology is surveyed, and gaps in modeling methodology are identified. The general requirements for a useful IAQ modeling and diagnostic tool are discussed, followed by a detailed outline of the specific research and development components required for the creation of such a tool.

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FOREWORD

This study was conducted for the U.S. Army Engineering and Housing Support Center (USAEHSC) under Project 4A162784AT41, "Military Facilities Engineering Technology"; Work Unit SA-AX1, "Human Habitability Requirements/IAQ." The USAEHSC technical monitor was Mr. C. Irby, CEHSC-F-UM.

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KEY ISSUES IN MODELING INDOOR AIR QUALITY FOR BUILDING DESIGN

1 INTRODUCTION

Background

Indoor air quality (IAQ) has been increasingly recognized as an important concern in recent years by building owners, managers, and occupants. Every year, researchers discover new connections between IAQ and occupant health, wellbeing, and productivity. Consequently, IAQ is now recognized to be an important concern in the design of a building. Good IAQ can be assured economically if potential problems are recognized during the design process instead of after completion. Because of the complex and subtle interrelationships between design and IAQ, however, architects and engineers currently design buildings without fully understanding the combined impact that their many decisions will have on the IAQ "built into" a design.

In order to recognize the possible IAQ problems that might be created by their decisions, architects and engineers—even if they are not IAQ experts—must be able to analyze the IAQ implications of a design at any stage of the design process. A computer-based IAQ modeling system would enable them to see the consequences of their decisions as they are being made instead of after design and construction are complete. By using such a modeling system during building design, potential IAQ problems can be addressed early in the building life cycle, when design changes are more feasible and less costly (see Figure 1). In contrast, fixing IAQ problems at the completion of the design process or after occupancy may require major redesign.

A useful modeling program would be able to predict important effects of IAQ, such as the likelihood of occupant complaints occurring in certain areas of the building, based on the quality of the environment that will result from the proposed design in those areas; the level of toxic off-gassing, based on the contaminant emission rates of the furniture and building materials; or the effect of various types of heating, ventilating, and air conditioning (HVAC) systems on the rate of biological contaminant growth. While an IAQ modeling system would offer the greatest benefits during the early design stages, the system should also be able to perform diagnostic analyses on existing buildings, working concurrently with redesign. The program should be able to analyze the building by using a set of computer-aided design (CAD) drawings in conjunction with information from an occupant IAQ questionnaire. For example, the system might diagnose an IAQ problem caused by biological contamination after analyzing occupant complaints in relation to the layout of the HVAC system.

The U.S. Army operates and maintains thousands of buildings on its installations worldwide, housing millions of military personnel and civilian employees. Since mission effectiveness is directly related to the health, well-being, and productivity of the people who work and live in Army buildings, the Army has a strong interest in promoting good IAQ. Furthermore, the Army's concern with cost effectiveness implies the demand for a comprehensive modeling tool that can help avoid IAQ problems and integrate good IAQ features into a building during the design phase. Currently, however, no such tool exists. This study is part of a research program by the U.S. Army Construction Engineering Research Laboratories (USACERL), a goal of which is to develop such a modeling tool.

Objective

The objective of this report is to identify key issues in the modeling of IAQ for application to a computer-based modeling system that can be used to integrate good IAQ features into a building throughout the design process.

Approach

Material about which aspects and parameters of IAQ to model is summarized from the findings of earlier USACERL research in this area. The basic requirements for a sophisticated IAQ prediction and diagnostic tool are then discussed. Current literature on modeling technologies is reviewed to determine the state of the art as it pertains to modeling IAQ for building design. Also considered are gaps in modeling methodology research that must be filled before technologies for a comprehensive IAQ modeling system can be developed. Finally, a detailed outline of the required research and development components for the IAQ prediction/diagnostic tool is presented.

Mode of Technology Transfer

This research program will result in the production and distribution of a software tool and documentation for Army architects and engineers. Training workshops or short courses are envisioned, and a user-support group may also be considered. Partnership arrangements such as Cooperative Research and Development Agreements (CRDAs) may also be appropriate.

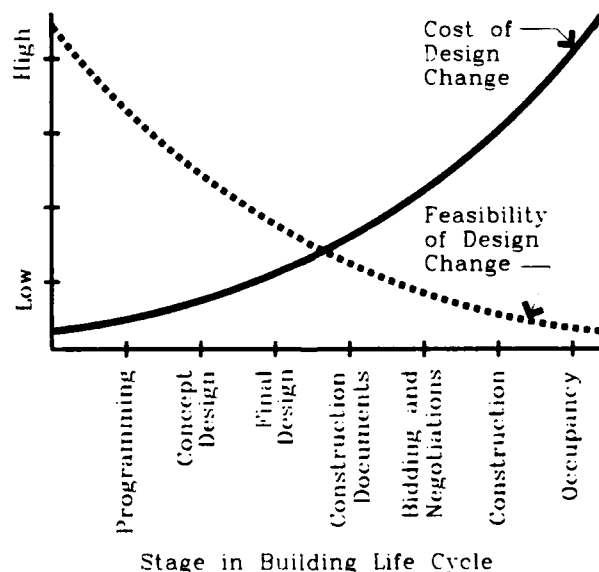


Figure 1. Cost and Feasibility of Design Change During Building Life Cycle.

2 REQUIREMENTS FOR DEVELOPING AN IAQ MODELING TOOL

Key IAQ Elements to Model

Many different contaminants can cause IAQ problems in buildings. However, a prohibitive amount of time and money would be required to investigate every possible cause of indoor air pollution (IAP). Most IAP can be detected by looking at 14 elements common to most IAQ problems—six reliable IAQ indicators and eight common contaminants.¹

The six reliable IAQ indicators are: occupant complaints, ventilation, mean radiant temperature, relative humidity, relative air velocity and movement, and odor. Occupant complaints of ill health, uncomfortable temperature, or unhealthy environment are often the first indicators of an IAQ problem. Ventilation—the amount of outside air entering a building—gives an indication of the amount of pollutant dilution that will occur. Temperature and humidity problems both can indicate a possible IAQ problem. Air velocity and movement indicate whether the flow of air to and throughout a space are adequate for providing good air quality. Odor is frequently an indication of a possible contaminant that may cause a problem.

The eight common contaminants responsible for most IAQ problems and resulting health hazards are: formaldehyde, volatile organic compounds (VOCs), respirable suspended particles (RSP), biological contaminants, asbestos, carbon monoxide, radon, and environmental tobacco smoke (ETS). Some of these are categories of contaminants; others are single, specific contaminants.

All of the above common pollutants may cause health problems if they are not eliminated or prevented. Formaldehyde can cause irritation of the skin and mucous membranes. At higher levels it may cause respiratory disease, asthma, and, eventually, cancer. VOCs irritate the eyes and lungs. RSP, which arise from poor cleaning, tobacco smoke, or poor-quality outside air, and can aggravate existing problems with radon or biological contaminants. Biological contaminants collect on dust particles and irritate the lungs, or cause diseases such as “humidifier fever”, asthma, or influenza. They can also irritate the mucous membranes and cause lethargy or shortness of breath. Asbestos fibers, when released from building materials, irritate the lungs and can cause asbestosis, mesothelioma, lung cancer, and gastrointestinal cancers. Asbestos increases the risk of cancer in smokers by a factor of 50. Carbon monoxide is toxic: it can cause headaches at low levels, and suffocation at higher levels. Radon can cause lung cancer. When the RSP level is high, radon is additionally dangerous because it adheres to the particles and is more readily embedded in the lungs. The irritation of ETS reduces employee productivity, and has been known to cause lung cancer and contribute to heart disease. ETS also aggravates the hazard of radon exposure by a factor of 5.

There are other, less common elements that can also contribute to an IAQ problem, but usually one or more of the 14 elements discussed above are directly linked to any IAQ problem. Therefore, each of them must be incorporated into any IAQ modeling program that will enable designers to design a “healthy” building by predicting (or diagnosing) conditions that may cause IAP.

¹ Eileen T. O'Connor, Don Kermath, and Michael R. Kemme, *Environmental Sensor Technologies and Procedures for Detecting and Identifying Indoor Air Pollution*, Interim Report (IR) P-92/07/ADA251882 (USACERL, March 1992).

Required Capabilities for an IAQ Prediction/Diagnostic Tool

An effective IAQ modeling tool must be capable of predicting problems during facility design—the preferred time to address such problems—and also diagnosing problems in existing buildings. Such a tool would work concurrently with automated drafting systems to form a powerful new design tool for architects and engineers. A prediction/diagnostic tool would work like an IAQ expert on the design team, ready to give implication warnings when the designer's decisions may result in poor IAQ. An effective tool will need to perform all the calculations, taking the necessary but repetitive groundwork out of the designer's scope of responsibilities, freeing him or her to concentrate on the act of design itself. Such a tool will provide calculations and guidelines that the designer can use as a foundation for efficiently achieving the main objective—the architecture or engineering of the building. Specific capabilities for an effective IAQ prediction/diagnostic tool should include the ability to:

- Consider all of the 14 IAQ indicators and contaminants listed above that are relevant to a particular design project
- Analyze CAD drawings for IAQ issues instantly and simultaneously with the designer
- Evaluate the HVAC system—the type of heating and cooling systems, the location of the chiller, the potential for stagnant water locations, etc.—and advise whether or not the chosen system will promote healthy IAQ
- Calculate the level of temperature, humidity, and air velocity that the building should have, and warn the designer when a decision may interfere with good IAQ
- Determine the necessary ventilation rate and help design a mechanical system that will adequately provide it
- Locate intake vents away from exhaust vents so polluted air will not be drawn into the fresh air intake
- Measure the rate of formaldehyde emission from furniture and building materials over time and make sure there is adequate ventilation to dilute the formaldehyde
- Evaluate the design to warn against any condition or configuration that might induce the accumulation of contaminants
- Evaluate the combined effect of all of the designer's decisions
- “Understand” building systems integration issues.

Most of these ideas cannot be adequately implemented with currently available technology. The IAQ prediction/diagnostic envisioned here would be sophisticated enough to consider and analyze building design in terms of the key IAQ issues specified at the beginning of this chapter. The tool would help the designer provide a healthy indoor environment without requiring that he or she be an IAQ expert.

Existing IAQ Modeling Tools

Modeling is used in many disciplines today, especially engineering. Most models are designed specifically for a certain process or application, such as predicting transformer operation, designing an electrical circuit, or analyzing the layout of a plumbing system. A majority of engineering models are computer programs.

Many modeling programs have been developed for IAQ applications, generally addressing specific subtopics of IAQ such as ventilation and air flow. The following sections summarize representative IAQ models from reports presented at the Fifth International Conference on Indoor Air Quality and Climate, 1990, in Ottawa, Ontario. Brief summaries of current IAQ model research by the U.S. Environmental Protection Agency (USEPA) are also presented.

Calculating Temperature and Velocity Fields in Ventilated Areas

According to a report by M. Ya. Poz,

There are two groups of models for calculating the parameters of air flows. The first uses Navier-Stokes equations for calculating air velocities in the space. These are versatile but very labor consuming. The second uses "adhesion" as follows. The space is divided into characteristic zones, and then solutions are calculated for each zone and adhered along the boundary of these zones. They can be applied when the specific nature of the motion of air flow in the space in question is (at least approximately) known.²

COMIS Air Flow Model

In an article on this model, Helmut E. Feustel reported that the Conjunction of Multizone Infiltration Specialists (COMIS) workshop,

... using a multi-national team, developed a multizone infiltration model on a modular basis. This model not only takes crack flow into account but also covers flow through large openings, single-sided ventilation, cross ventilation and HVAC-systems. COMIS can also be used as a basis for future expansion in order to increase the ability to simulate buildings.

The latest development in infiltration modeling is the COMIS model. In a twelve-month period ten scientists from nine countries developed a multizone model on a modular basis. Because of its modular structure COMIS is designed to expand its capability to simulate buildings. To accomplish a user-friendly program special emphasis was given to the input routines. Support of the international group, working together at Lawrence Berkeley Laboratory, by the Air Infiltration and Ventilation Center of the International Energy Agency [are] likely to ensure the wide distribution of this model to all interested parties. COMIS can be used as a stand-alone infiltration model with input and output features or as an infiltration module for thermal building simulation programs. It also serves as a module library.³

² M. Ya. Poz, "Physio-Mathematical Models for Calculating Temperature and Velocity Fields in Ventilated Areas," *Indoor Air '90—Proceedings of the 5th International Conference on IAQ and Climate*, Vol 4 (Ottawa, Ontario, 1990), p 89.

³ Helmut E. Feustel, "The COMIS Air Flow Model—A Tool for Multizone Applications," *Indoor Air '90*, pp 121, 123.

Computer-Aided Facilities Diagnostics

Alan Hedge and Dana Ellis described the new Computer-Aided Facilities Diagnostics (CAFD) software as follows:

Studies of office environmental problems to date have provided only a sketchy picture of the causes and cures of the "sick" building syndrome. In part this may reflect the difficulty of interpreting survey results presented as summary statistics which may be devoid of important spatial information...[CAFD] has been developed to graphically combine survey data and building floor plans. The potential benefits of CAFD in diagnosing building problems will be discussed.

CAFD works by importing digitized floor plans from a wide variety of computer drawing/drafting (CAD) packages, and this information is then combined with a database containing either the survey response information, or environmental information, or indeed any database of spatially distributed information. With this tool the user can interact with the database to examine the spatial distribution of responses in an office. The software allows users to specify the questions of interest and then it plots the distribution of responses to these questions. To assist with interpretation, responses are color-coded, e.g., better values can be shades of blue and worse values shades of red. To illustrate the potential benefits of using an approach like this, results from a survey of a suspected "sick" building [are] presented. Descriptive statistical analysis of these [are] compared with analysis of the data using the CAFD software.⁴

IAQ Model Review

James Axley prepared a review of all the IAQ models that the National Institute of Science and Technology (NIST) has developed. He summarized the capabilities of these programs as follows:

- CONTAM86: Nonreactive, single contaminant dispersal analysis for specified airflows; steady-state response and time constant analysis for steady flow conditions; dynamic response analysis for arbitrary flow and excitation time histories
- CONTAM87: As above for reactive, multiple-contaminant dispersal analysis adding reaction and one-dimensional convection-diffusion finite elements
- AIRNET: Steady-state airflow analysis for specified temperature fields and pressure fields (e.g., due to wind), including all flow analysis elements above, except the crack element
- DTAM1: Thermal analysis; steady-state response and steady harmonic response for steady and steady harmonic excitation; dynamic response analysis for arbitrary excitation time histories
- CONTAM88: An integration of CONTAM87 and a reduced-capability version of AIRNET
- NBSAVIS: A building description interface used as a preprocessor to CONTAM88

⁴ Alan Hedge and Dana Ellis, "Computer-Aided Facilities Diagnostics: A New Software Tool for Investigating Indoor Environmental Problems," *Indoor Air* '90, pp 127-128.

- DTFAM: Coupled flow/thermal analysis currently under development: an integration of DTAM1 and a reduced-capability version of AIRNET; steady state and quasi-dynamic analysis capabilities.⁵

Multichamber Consumer Exposure Model

M. Koontz et al reported on the new Multichamber Consumer Exposure Model (MCCEM), developed for the U.S. Environmental Protection Agency (USEPA).

[This model] is a user-friendly computer program that estimates indoor concentrations for, and individual exposure to, chemicals released in indoor environments such as residences. Concentrations can be modeled in as many as four chambers or zones of a building. Model inputs include air infiltration and interzonal airflow rates, time-varying emission rates in each zone, outdoor concentrations, first-order decay rate, and location of an individual over time. Options available with the model include Monte Carlo simulation, sensitivity analysis, estimation of the percent of time exposed above a user-specified level of concern, and estimation of lifetime average daily exposure (LADE).⁶

Calculating Individual Exposure

A report by L.E. Sparks and W.G. Tucker introduced two more IAQ models:

A model for calculating individual exposure to indoor air pollutants from sources...is designed to calculate exposure due to individual, as opposed to population, activity patterns and source use. The model uses data on source emissions, room-to-room air flows, air exchange with the outdoors, and indoor sinks to predict concentration-time profiles for all rooms. The concentration-time profiles are then combined with individual activity patterns to estimate exposure. The agreement between predicted concentration-time profiles and experimental data is excellent.

An...IAQ computer model, INDOOR, was developed to use emission characteristics of sources to predict in-room pollutant concentrations. INDOOR's predictions for several sources have been verified by experiments conducted in an IAQ test house, and emission characteristics have been determined using techniques in Tichenor.

INDOOR, however, does not allow calculation of individual exposure due to a given source and personal activity pattern. The ability to estimate individual exposure is necessary before guidance on exposure reduction can be given. Therefore, a new model, EXPOSURE, that allows analysis of exposure due to indoor sources (given pollutant source characteristics and individual activity patterns) was developed.⁷

Specification of Indoor Air Model Characteristics

Bruce Weir et al reviewed nine IAQ models. Discussed first were the possible capabilities of the models, followed by specifics of each of the nine individual models. Possible capabilities cited were:

1. Level 1—Given personal exposure data, can estimate the population exposure distribution for the population as a whole and for particular subgroups

⁵ James Axley, "IAQ Model Review," *Indoor Air '90*, p 119.

⁶ M. Koontz et al, "The Multichamber Consumer Exposure Model (MCCEM)," *Indoor Air '90*, p 145.

⁷ L.E. Sparks and W.G. Tucker, "A Computer Model for Calculating Individual Exposure Due to Indoor Air Pollution Sources," *Indoor Air '90*, p 213.

2. Level 2—Given microenvironment concentrations and activity patterns, can estimate population exposure. This includes concentrations calculated as part of the model
3. Level 3—
 - a. Given air exchange rates, removal rates, source strength, and outdoor concentrations, can estimate microenvironment concentrations
 - b. Can optionally calculate or sample air exchange rates from a data set
 - c. Can estimate source strength based on emission rate, load factor, and source duration
 - d. Can estimate source strength for combustion sources, consumer products, material sources, and water
4. Can analyze both gaseous and particulate pollutants
5. Can estimate for several averaging times
6. Can integrate exposures in several different microenvironments
7. Can assess the effects of potential mitigation measures
8. Can estimate exposure by noninhalation pathways
9. Can operate on a PC with a user-friendly interface.

The following are descriptions of the nine individual models:

1. National Ambient Air Quality Standards Exposure Model (NEM)—capabilities 1, 2, 3a, 3c, 3d, 4, 5, 6, 7, 8. NEM is an urban-scale exposure model developed for USEPA to estimate population exposure to criteria pollutants. Diurnal patterns of movement between six microenvironments, such as outdoors, inside a home, inside an office, etc., are defined for each age and occupation group. Model results include hourly exposures for each census district for each age-occupation cohort. Systems Applications has enhanced NEM for ozone exposure, NEM/SAI with the addition of an explicit indoor air quality model (also a stand-alone model; see PAQM). A version of this model has been developed for the South Coast Air Quality Management District (Los Angeles, California) as SCREAM-II (South Coast Risk and Exposure Assessment Model).
2. Personal Air Quality Model (PAQM)—capabilities 1, 2, 3a, 3c, 3d, 4, 5, 6, 7, 8. PAQM was developed by Systems Applications to estimate the indoor exposures due to population groups' daily activities. PAQM uses 56 different population groups with distinct activity patterns for weekdays, Saturdays and Sundays. Eleven different microenvironments are used with a single-compartment indoor module. Building parameters and source terms are user-defined and optionally time-varying.
3. Regional Human Exposure Model (REHEX)—capabilities 1, 2, 4, 6. REHEX, developed by Winer et al, is similar to NEM except that it uses frequency distributions of air quality data for each hour of the day, rather than a time series. This enhances computational efficiency,

but prohibits estimations of multiperiod averages. The model addresses three microenvironments: outdoors, in-transit, and indoors. Indoors and in-transit concentrations are estimated as in NEM, i.e., as a fraction of the outdoor concentration plus contribution from indoor sources. Population mobility among exposure districts is included. This model's nine age-occupation groups are divided into numerous subgroups, each with a different activity pattern. Thus, variability in activity patterns is more detailed. The likelihood of capturing the upper tail of the exposure distribution associated with an atypical activity is thus increased.

4. **Simulation of Human Activity and Pollutant Exposure Model (SHAPE)**—capabilities 1, 2, 4, 5, 6. SHAPE, developed by USEPA, uses activity pattern data in conjunction with microenvironment concentrations. SHAPE's activity patterns may be either deterministic or generated through a Monte Carlo sampling process. The authors state that application of the sampling option to other than carbon monoxide exposures requires "more extensive analysis of the database than has been carried out thus far."⁸ The microenvironment concentrations for each period are sampled from an empirical or statistical frequency distribution. The population is tracked sequentially so that multi-period average exposures may be estimated. The authors note that the assumed time-independence of microenvironment concentrations may underestimate the upper tail of the exposures.
5. **Macromodel for Assessing Residential Concentrations of Combustion Generated Pollutants (MACROMODEL)**—capabilities 3a, 3b, 3c, 4, 7. The MACROMODEL estimates indoor air concentrations, but not exposures. It contains detailed modeling of combustion sources. It assumes well mixed and steady-state air masses, which may underestimate the upper tail of the exposure distribution. The authors note that open windows and doors are not addressed, so summer air exchange may be underestimated and concentrations overestimated. It uses a fixed averaging time of 1 week.
6. **Indoor Air Quality Model Personal Computer Version (IAQPC)**—capabilities 3a, 3c, 3d, 4, 5, 7, 9. The IAQPC model, developed at USEPA by Sparks and others, also addresses indoor air quality and not exposure. It estimates concentrations in multicompartments structures on the basis of air exchange, removal rate, source strength, and outdoor concentrations. Air exchange parameters are user-defined rather than sampled. The actual airflow distribution is determined according to pressure balance equations, but not on the basis of external factors. The model allows for two modes of air flow (i.e., HVAC system on or off) with user-defined switching times. Source strength is modeled for a number of different source types, as is removal due to reactivity of deposition with the possibility of re-emission. Like PAQM, the timing of combustion source emissions is user-defined rather than estimated from building parameters and external conditions. However, tobacco smoke emissions are randomly distributed within each particular hour to simulate smoking behavior, which prohibits reproducibility of model results. Concentration-time profiles are determined as well as user-defined. Mitigation measures affecting source duration, load, air exchange, or HVAC functioning may be assessed. The model employs a user-friendly menu interface.

⁸ Bruce Weir et al, "Specification of Indoor Air Model Characteristics," *Indoor Air '90*, p 231.

7. CONTAM—capabilities 3a, 3c, 3d, 4, 5, 7. CONTAM also estimates the microenvironment concentration based on air exchange rate, removal rate, source strength, and outdoor concentration for a multicompartment structure. Air exchange rates are determined from user-defined flow rates rather than from sampled parameters or calculations. Source strength is user-defined and time-variable. Pollutants may be removed or generated by chemical transformations or deposition at user-defined rates. Mitigation measures affecting building configuration, airflow rates, HVAC system parameters, source emission rates, or source emissions duration may be assessed. The model may find a steady state or the time trajectory of concentrations. Multiperiod averaging is possible. CONTAM also uses a well-mixed assumption. It is not an exposure model.
8. Indoor Air Quality Model (IAQ)—capabilities 2, 3a, 3c, 5, 6, 7. McKone's IAQ model estimates the concentration of VOCs from contaminated tap water in a three-compartment structure on the basis of source strength and air exchange. It also estimates lifetime average inhalation exposure, using simplified activity data and three microenvironments: shower, bathroom, and rest of the house. Air exchange is calculated from user-defined air residence times and compartment volumes. Sources are from user-defined emissions and timing. Multiperiod exposure concentrations would be possible with hour-by-hour activity patterns. Mitigation measures affecting source duration, emission rates, and air exchange could be investigated.
9. California Institute of Technology Indoor Model (CIT)—capabilities 3a, 3c, 4, 5, 7. CIT is designed to estimate concentrations of chemically reactive compounds or particulate matter in one or more compartments on the basis of air exchanges, removal and generation, source strength, and outdoor concentrations. Air exchange is calculated from user-defined airflows. Source exchange rates and source strength are included. Both models use a well-mixed assumption. In the reactive version, pollutants may be generated or transformed on the basis of chemical kinetics. These relationships are only available for the species included. In the particulate version, size transitions and deposition by aerodynamics are treated. Multiperiod averaging is possible for both versions.⁹

IAQ Modeling Research by USEPA

IAQ Macromodel for Assessing IAP from Combustion Appliances. The purpose of this research is to develop and validate a macromodel for predicting IAP concentrations. A draft report on this system has been completed.¹⁰

IAQ Model. The purpose of this research is to verify NIST models and improve the user friendliness of IAQ models. Publication of a final report was expected in fall, 1990.

IAQ Macromodel Development. This macromodel is intended to estimate residential indoor pollutant concentration distributions in the United States. A journal article and summary report¹¹ on a combustion macromodel (carbon dioxide, nitrous oxide, and RSP) were to be completed 1990; a report on a macromodel approach to PAHs, sulfur dioxide, and VOCs was expected in early Fiscal Year (FY) 91.

⁹ Bruce Weir et al.

¹⁰ G.W. Traynor et al, *Macromodel for Assessing Residential Concentrations of Combustion Generated Pollutants: Model Development and Selected Sensitivity Analyses*, LBL 28450 (Lawrence-Berkeley Laboratory, February 1990).

¹¹ G.W. Traynor et al.

Indoor Air Pollution and Building Airflow Models. The purpose of this research is to develop generalized simulation programs that account for air movement and contaminant dispersal within buildings due to generation, dilution, reaction, adsorption, and other mechanisms. Contaminant adsorption models have been developed. NBSAVIS and CONTAM88 are available for multizone airflow and contaminant modeling. Professional series of CONTAM was to be available at end of FY 90.

Three-Dimensional Modeling of Room Air Motion. The purpose of this research is the development and application of computer models to predict three-dimensional velocity fields and contaminant concentrations within ventilated spaces. The model is intended to produce information for ventilation system design. The computer model has been developed and is being applied to various office configurations. Validation efforts are in progress.¹²

Modeling Methodologies: Issues and Research Needs

A number of IAQ-related subjects require further research before models can be developed. Current technology is not advanced enough to provide all of the information a comprehensive model would require. At a symposium on air quality sponsored by the National Science Foundation (NSF),¹³ various IAQ modeling methodologies were discussed, as well as research that still needs to be done within each area. The following general needs were identified as gaps in current air quality knowledge and methodology:

1. Technology to provide detailed information on temperature and air quality is needed at different locations within rooms so the information can be fed into the computer control system and used as a basis for adjusting the HVAC system.
2. Researchers need to know how adjustments affect a room's environment at different points.
3. Research is needed to discover what happens when:
 - People, animals, and objects move about in rooms
 - The weather changes
 - Locations of thermal and contaminant sources shift within rooms
 - Desired conditions fluctuate at different places and times within rooms.

For this symposium, macromodels were used to determine the flow of air and contaminants from one zone to another within a building through predetermined or known discrete flow paths. Micromodels were used to examine the details of air and contaminant movement within individual air spaces or zones.

In the area of mathematical modeling, research needs were identified for macro- and micro-level modeling, on-line modeling for control of HVAC systems, contaminant sources and sinks, physical modeling, and descriptive methods.

¹² *Current Federal Indoor Air Quality Activities*, EPA 400/10-90/006 (USEPA, October 1990).

¹³ "Building Systems: Room Air and Air Contaminant Distribution," University of Illinois at Urbana-Champaign, 5-8 December 1988.

Macro-Level Modeling

For macro-level modeling, the following observations were made:

1. It is used to predict the time and spatial variation of global measures of airflow, contaminant dispersal, and heat transfer in whole-building systems
2. Macro-level models are currently available for contaminant dispersal analysis, steady airflow analysis, and thermal analysis of whole-building systems, moisture transfer and HVAC system analysis in subsystems or parts of building systems
3. These models provide no in-room detail
4. They are simple, numerically straightforward, computationally nondemanding, and easy to use
5. Contaminant dispersal analysis is limited by
 - a. The need to know all flows in the system accurately to complete the analysis
 - b. The completeness and accuracy of contaminant source or sink models used to drive the analysis
6. Limitations of flow analysis include:
 - a. The accuracy of the flow "laws" used to characterize the discrete flow paths
 - b. The accuracy of the temperature distribution that must be known to begin the solution (because it determines buoyant effects)
 - c. The accuracy in modeling the pressure distribution when wind acts on the building
7. Integrating macro- and micro-level modeling would provide detailed information for parts of a building system while still taking whole-system interaction into account
8. The micro/macro- level modeling approach may be possible for contaminant dispersal, moisture transfer, and thermal analysis, but its application to flow analysis is yet untried and may be of limited value
9. Integration of macro-level models of different classes can also be useful. In particular, building envelope thermal models have been integrated with HVAC system models to account for HVAC system-building interaction
10. Macro-level models for analyzing contaminant dispersal need to provide greater resolution of detail within single rooms
11. Researchers need to develop source models that can be incorporated into macro-level contaminant dispersal analysis or sink removal characteristics on the state parameters governing dispersal within a building.

The areas of macro-level modeling still requiring significant research are:

1. Contaminant dispersal modeling for single rooms
2. Source and sink modeling
3. Validation of models
4. Improved prediction of wind-driven pressure distribution on buildings
5. Coefficients for internal surface heat and mass transfer
6. Integration of thermal analysis models
7. Integration of macro- and micro-level flow analysis.

Micro-Level Modeling

Micro-level modeling is used primarily to study spatial distribution of air temperature, velocity, and contaminant concentrations in a room. The areas of micro-level modeling still needing to be researched are:

1. Flexible geometry capabilities
2. Improved boundary condition functions for momentum and heat flux
3. Turbulence closure models
4. Application of expert systems to CFD models
5. Validation of models
6. Application of models to practical ventilation problems.

On-Line Modeling for HVAC Control

For this type of modeling, an adaptive control algorithm takes into account the variations over time of internal gas, heat, and moisture that room occupants produce, as well as the environmental conditions they desire. Areas still needing to be researched include:

1. Control based on air velocities and turbulence
2. Criteria for choosing data for model database volumes
3. Development of scaling theory for dynamic systems.

Containment Sources and Sinks

The areas of this topic still needing to be researched are:

1. Modeling concepts for sources, sinks, and interactions
2. Data on the behavior of pollutants at sources and sinks as functions of environment and other factors
3. Application of atmospheric science approaches to rooms.

Physical Modeling

The areas of physical modeling that still need significant research or development are:

1. A standardized data reporting format and a clearinghouse (database) for the data
2. Experimentation to develop information for:
 - a. ADPI, including modification for heating
 - b. Coefficients and parameters for mass-balance models
 - c. Generation of contaminants within spaces
 - d. Contaminant removal and sink rates
 - e. Diffuser performance characteristics
 - f. Visualization techniques
 - g. Scaling theory
 - h. Risk analysis
3. Validation methods for newly developed models
4. Data and tools to predict end-use IAQ
5. Similitude modeling techniques for "real rooms" with internal heat sources and obstructions
6. Data on performance of contaminant removal and containment systems.

Descriptive Methods

Short-term research needs include:

1. Identification of typical sources of IAP
2. Improved descriptive models of thermal comfort, air movement, and diffuser characteristics

3. Design methods for isolating contaminant sources for smoking areas, fume hoods, and disease organisms
4. More precise definitions of ventilation efficiency
5. Techniques for flow visualization
6. Links between air and contaminant distribution
7. ADPI-type design techniques for heating systems
8. Effects of multiple environmental stressors on human health
9. Key issues for proper building operation

Long-term needs include:

1. More knowledge about the relationship of comfort parameters to productivity
2. Integration of air distribution and contaminant control systems
3. Knowledge-based systems for system design and operation
4. Multidisciplinary surveys in occupied buildings
5. Design techniques that include furniture, people, lighting, etc.
6. Knowledge about the effects of supply air diffusers on hood spills
7. Knowledge of forces causing intrazonal and interzonal movement of pollutants
8. Better understanding of the cause and comfort effect of large eddies of air in rooms
9. Personal climate control systems
10. Whole-building performance diagnostic methods.

USEPA Methodology Research

Current USEPA research into modeling methodologies includes the following specific projects:

1. Consumer Exposure Methodology and Guidelines for Collection of Data Pertaining to Inhalation Exposure in Residential Buildings. The purpose of this research is to present methods for assessing consumer exposure to IAP, including models to estimate indoor concentrations. Different approaches to assess exposure to toxic chemicals in homes is described. A report on

methodology available¹⁴ and draft guidelines on approaches for collecting data related to in-house inhalation exposure are under review.¹⁵

2. PFT (perfluorocarbon tracer) Database. This research is intended to improve methods for modeling exposure to indoor air contaminants in homes. The collection of an extensive data set of air exchange rates and interzonal air flows in homes was completed in 1990.
3. Air Infiltration Research. The goal of this work is to develop methods for modeling and measuring infiltration and interzonal air flows. An international collaborative research program on air flow modeling is currently under consideration.

Dynamic Research Needs

The modeling tools and methodologies discussed here are representative of the work being conducted in IAQ research and development circles. As this research advances, both within USACERL and other Government and non-Government organizations, it is likely to reveal additional gaps in knowledge and technology, even as the gaps discussed here are filled. By specifying a set of minimum acceptable requirements for an effective integrated IAQ modeling system, however, the scope of necessary research may be defined to most effectively focus resources on the creation of such a system.

Research Requirements for Development of the Prediction/Diagnostic Tool

The following outline lists the research needs to be met in order to fully develop an effective, integrated IAQ prediction/diagnostic modeling tool like the one discussed in the second section of this chapter:

- I. Diagnostics
 - A. Provide guidance on performing inspections
 1. Air flow—overall and local
 2. Ventilation—overall and local
 3. HVAC intake and exhaust
 4. Source identification
 5. Pollutant measurement
 6. Processing input from interview with building management and maintenance personnel
 - B. Post-Occupancy Evaluation
 1. Processing input about occupant perception of IAQ
 2. Occupant symptoms typically related to IAQ
 3. Processing input from occupant interview
 - C. Products
 1. Guidance documents
 2. Integrated IAQ environmental sensors
 3. User guide to diagnostics

¹⁴ "Methods for Assessing Exposure to Chemical Substances," *Methods for Assessing Consumer Exposure to Chemical Substances*, Vol 7 (USEPA, Office of Toxic Substances, April 1987).

¹⁵ GEOMET Technologies, Inc., *Guidelines for Collection of Data Pertaining to Inhalation Exposures in Residential Buildings*, draft report (USEPA, Office of Toxic Substances, 11 August 1989).

- I. Source Emissions/Sinks/Concentrations**
 - A. Outdoor contributions**
 - B. Construction materials and furnishings**
 - C. Emissions related to occupant use**
 - 1. Office machinery (copiers, graphic arts, combustion sources, etc.)
 - 2. Special uses (laboratories, cafeterias, etc.)
 - 3. Smoking
 - 4. Bioeffluents
 - D. Emissions related to operations and maintenance (O&M)**
 - 1. Cleaning products
 - 2. Pesticide application
 - 3. Maintenance activities (vacuuming, painting, welding, roofing, etc.)
 - 4. Biogenic emissions from HVAC components (cooling towers, humidifiers, etc.)
- II. Source pollutant measures: identify to prevent IAQ problems, diagnose existing problems, and measure the success of mitigation.**
 - A. IAQ elements measured**
 - 1. Poor ventilation (carbon dioxide)
 - 2. ETS
 - 3. Formaldehyde
 - 4. VOCs
 - 5. Biological contaminants (total bacterial, fungal, spore counts)
 - 6. Radon
 - 7. Asbestos
 - 8. Products of combustion (carbon monoxide, nitrous oxide, sulfur dioxide, RSP)
 - 9. RSP
 - B. Products**
 - 1. IAQ emissions inventory system (database of sources and emissions)
 - 2. Operation and maintenance guidance
- III. Mitigation—affordable and effective indoor air contaminant remediation**
 - A. Source reduction**
 - B. Avoidance**
 - C. Maintenance**
 - 1. Predictive
 - 2. Preventive
 - D. Ventilation**
 - E. Air cleaning techniques**
 - 1. Filtration
 - 2. Absorption
 - 3. Dilution
- IV. Design**
 - A. New construction**
 - B. Remodeling, reuse, and renovation**
- V. Indoor air contaminant concentration**
 - A. Mass balance**
 - B. Dispersion**

VII. Concurrent engineering

- A. Techniques**
- B. Hardware**
- C. Software**

VIII. Environmental sensor technologies

- A. Sensing**
- B. Monitoring**
- C. Control devices**
- D. Organic and mechanical sensors**

USACERL is developing a major research plan that will ultimately produce an IAQ modeling tool such as the one described here. This plan will organize and prioritize the many aspects of IAQ-related research that must be conducted, including activities such as technology transfer, education and training, and marketing. The IAQ-related activities of other Government and non-Government agencies will play an important role in the USACERL research plan: coordination with organizations doing research related to the overall goal will help USACERL focus resources on specific unmet needs and avoid duplication of effort.

3 SUMMARY

This report has discussed key issues in the development of a computer-based IAQ modeling system for building design. The system's greatest benefit would be to help integrate healthy IAQ into a building during the design stage, when it is least costly to do so, but it could also be used as a diagnostic tool for existing buildings. The system would address the 14 common IAQ indicators and contaminants associated with the majority of IAQ problems. Existing IAQ modeling technology will be useful in developing the system, but a number of gaps in IAQ modeling methodology must be filled before other required technologies can be developed. The specific research and development requirements for a sophisticated IAQ prediction and diagnostic tool were outlined, and it was noted that the broad scope of this work would require coordination with other Government and private-sector organizations doing related research.

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ABBREVIATIONS AND ACRONYMS

ADPI	Air Diffusion Performance Index
AIRNET	Airflow Network
CAD	computer-aided design
CAFD	Computer-Aided Facilities Diagnostics
CFD	Computation Fluid Dynamics
CIT	California Institute of Technology Indoor Model
COMIS	Conjunction of Multizone Infiltration Specialists
CRDA	Cooperative Research and Development Agreement
DTAM	Discrete Thermal Analysis Method
ETS	environmental tobacco smoke
FY	Fiscal Year
HVAC	heating, ventilating, and air conditioning
IAP	indoor air pollution
IAQ	indoor air quality (also Indoor Air Quality Model)
IAQPC	Indoor Air Quality Personal Computer Version
LADE	lifetime average daily exposure
MCCEM	Multichamber Consumer Exposure Model
NEM	National Ambient Air Quality Standards Exposure Model
NIST	National Institute of Standards and Technology
NSF	National Science Foundation
O&M	operations and maintenance
PAH	Polycyclic Aromatic Hydrocarbons
PAQM	Personal Air Quality Model
PC	personal computer

PFT	perfluorocarbon tracer
REHEX	Regional Human Exposure Model
RSP	respirable suspended particles
SAI	Systems Applications, Inc.
SCREAM	South Coast Risk and Exposure Assessment Model
SHAPE	Simulation of Human Activity and Pollutant Exposure Model
USACERL	U.S. Army Construction Engineering Research Laboratories
USAEHSC	U.S. Army Engineering and Housing Support Center
USEPA	U.S. Environmental Protection Agency
VOC	volatile organic compound

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